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The electronic structure and magneto-optical Kerr effect of Tm monochalcogenides.

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The optical and magneto-optical (MO) spectra of Tm monochalcogenides are investigated theoretically from first principles, using the fully relativistic Dirac LMTO band structure method. The electronic structure is obtained with the local spin-density approximation (LSDA), as well as with the so-called LSDA+U approach. In contrast to LSDA, where the stable solution in TmTe is a metal, the LSDA+U gave an insulating ground state. LSDA+U theory predicts the thulium ion in TmTe to be in an integer divalent state. It also shows a gradual decreasing of the energy gap with reducing of the lattice constant. LSDA+U theoretical calculations produce a similar energy band structure in TmS and TmSe, with twelve $4f$ bands fully occupied and hybridized with chalcogenide p states. The 14th f hole level was found to be completely unoccupied and well above the Fermi level and a hole 13th f level is partly occupied and pinned at the Fermi level. The occupation number of the 13th f level is equal to 0.12 and 0.27 in TmS and TmSe respectively (valence 2.88+ and 2.73+). Such an energy band structure of thulium monochalcogenides describes well their measured BIS, XPS and UPS spectra as well as the optical and MO spectra. The origin of the Kerr rotation realized in the compounds is examined.